

Amendments to the Claims

Claims 1-73 (withdrawn)

Claims 74-75 (cancelled)

Claim 76 (currently amended): The method of claim 74 128, wherein said step of determining a relationship comprises the step of determining $\hat{y}_i = f(x_{ij})$, where x_{ij} denotes a whole molecule parameter, i ranges from 1 to n where n represents the number of first test peptides in the plurality thereof, j ranges from 1 to d where d represents the number of whole molecule parameters, and \hat{y}_i represents an estimate of the measured first indicia of the activity of the plurality of first test peptides.

Claims 77-81 (cancelled)

Claim 82 (currently amended): The method of claim ~~81~~ 128, wherein said space-filling design expands less than all of the first test peptides into their constituent compound isomers ~~further comprising the step of expanding less than all of the candidate peptides determined in said representing step into their constituent compound isomers using a space-filling design.~~

Claim 83 (currently amended): The method of claim 74 128, wherein said whole molecule parameter is selected from the group consisting of total charge, molecular weight, isoelectric point and total dipole moment.

Claim 84 (currently amended): The method of claim 74 128, wherein said whole molecule parameter is selected from the group consisting of total charge, molecular weight, isoelectric point and total dipole moment, and further wherein said sequence specific parameter is selected from the group consisting of isotropic surface area, electronic charge index and hydrophobicity.

Claim 85 (currently amended): The method of claim 74 128, wherein said sequence-specific parameter is selected from the group consisting of isotropic surface area, electronic charge index and hydrophobicity.

Claim 86 (currently amended): The method of claim 74 128, wherein said whole molecule parameter is molecular weight and at least one additional parameter selected from the group consisting of total charge, isoelectric point, total dipole moment, isotropic surface area, electronic charge index, and hydrophobicity.

Claim 87 (currently amended): The method of claim 74 128, wherein the activity is binding to a receptor.

Claim 88 (currently amended): The method of claim 74 128, wherein the activity is enhancement or inducement of a biological activity in a cell.

Claim 89 (currently amended): The method of claim 74 128, wherein the activity is inhibition or prevention of a biological activity in a cell.

Claim 90 (original): The method of claim 88 or claim 89, wherein the cell is a cell cultured in vitro.

Claim 91 (currently amended): The method of claim 90, wherein the step of measuring ~~an~~ the indicia said activity comprises:

forming a plurality of culture media that each contains a respective test peptide from the plurality thereof; and

adding each of the plurality of culture media to a respective cell culture to form a plurality of cell cultures each containing a respective culture medium containing a respective first test compound.

Claim 92 (currently amended): The method of claim 74 128, wherein the activity is inhibition or prevention of activation of a receptor.

Claim 93 (currently amended): The method of claim 74 128, wherein the activity is enhancement or inducement of activation of a receptor.

Claim 94 (currently amended): The method of claim 74 128, wherein the first test peptide library consists of peptides having a length of no less than four amino acids.

Claim 95 (currently amended): The method of claim 74 128, wherein the first test peptide library consists of peptides having a length of no more than ten amino acids.

Claims 96-127 (withdrawn)

Claim 128 (new): A method of identifying a peptide with a desired activity having an indicia that satisfies a test requirement, the method comprising the steps of:

constructing a first test peptide library comprising a plurality of first test peptides by means of a space-filling design, wherein the length of said first test peptides comprises no greater than twenty amino acids, and wherein said first test peptides are characterized by a first parameter and a second parameter, said first parameter being a whole molecule parameter and said second parameter being a sequence-specific parameter;

determining an activity, having an indicia, of said plurality of first test peptides;

measuring the indicia of said activity of said plurality of first test peptides;

determining a relationship between said indicia of said activity, said first parameter, and said second parameter;

calculating an estimated indicia for each first test peptide in said first test peptide library using said determined relationship;

setting a test requirement, based on a desired activity, having a test indicia range;

selecting a second test peptide library comprising at least one second test peptide, wherein each second test peptide is a first test peptide having an estimated first indicia that satisfies said test requirement;

determining the indicia of said at least one second test peptide; and

identifying at least one second test peptide having an indicia that satisfies said test requirement.

129 (new) The method of claim 128 further comprising the steps:

selecting a subgroup of first test peptides, from said test peptides, having an indicia that satisfies said test requirement; and

expanding said first test peptides from said subgroup into their constituent compound isomers using a space-filling design to identify candidate peptides having said indicia of activity;

wherein:

said step of calculating comprises a step of calculating an estimated indicia for each candidate peptide using said determined relationship, and

said step of selecting a second test peptide library comprises a step of selecting a second test peptide library containing at least one candidate peptide having an estimated indicia that satisfies said test requirement.

130. (new) A method of identifying a peptide with a desired activity having an indicia that satisfies a test requirement, the method comprising the steps of:

identifying initial peptides having a length no greater than twenty amino acids, and wherein said initial peptides are characterized by a first parameter and a second parameter, said first parameter being a whole molecule parameter and said second parameter being a sequence-specific parameter;

selecting a plurality of test peptides from said initial peptides to form a first test peptide library using a space filling design;

measuring the indicia of an activity of said plurality of test peptides;

determining a relationship between said measured indicia, said first parameter, and said second parameter of said plurality of test peptides;

calculating an estimated indicia for each initial peptide using said determined relationship;

setting a test requirement based on a desired activity, said test requirement having a test indicia range;

selecting a second test peptide library comprising at least one initial peptide having an estimated indicia that satisfies said test requirement;

measuring the indicia of said at least one second test peptide; and

identifying at least one second test peptide having a measured indicia that satisfies said test requirement.

131. (new) The method of claim 130, wherein said step of selecting a plurality of test peptides is performed using a space-filling design that applies a distance function.

132. (new) The method of claim 130, wherein the number of initial peptides in said second test peptide library exceeds a predetermined threshold suited for performing said measuring step, and prior to conducting the step of measuring, performing the steps:

selecting a plurality of new peptides from said first test peptide library to form a new test peptide library using a space filling design;

determining a new relationship between said measured indicia, said first parameter, and said second parameter;

calculating an estimated indicia for each initial peptide using said new determined relationship;

selecting a new second test peptide library comprising at least one initial peptide having an estimated indicia that satisfies said test requirement; and

repeating said steps of selecting a plurality of new peptides, determining a new relationship, calculating an estimated indicia, and selecting a new second test peptide library until the number of initial peptides in said new second test peptide library does not exceed the predetermined threshold.

133. (new) The method of claim 132, further comprising, prior to performing said step of selecting, a step of adjusting said test requirement by a desired value for improving results of said step of selecting a new second peptide library.

134. (new) The method of claim 130, wherein the number of initial peptides in said second test peptide library exceeds a predetermined threshold suited for performing said measuring step, and prior to conducting the step of measuring, performing the steps:

selecting a plurality of new peptides from said first test peptide library to form a new test peptide library using a space filling design;

determining a new relationship between said measured indicia, said first parameter, and said second parameter;

calculating an estimated indicia for each initial peptide using said new determined relationship;

selecting a new second test peptide library comprising at least one initial peptide having an estimated indicia that satisfies said test requirement; and

repeating said steps of selecting a plurality of new peptides, determining a new relationship, calculating an estimated indicia, and selecting a new second test peptide library until the measured indicia of at least one of the initial peptides in the second test peptide library satisfies a predetermined threshold.